

Riesling acetal

Inchi:	InChI=1S/C13H20O2/c1-10(2)6-5-7-11(3)13(10)9-8-12(4,14-11)15-13/h5,7H,6,8-9H2,1-4
InchiKey:	QXHORPLJTIHQGR-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CC12CCC3(O1)C(C)(C)CC=CC3(C)O2
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	44.68	kJ/mol	Joback Method
hf	-271.17	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.027		Crippen Method
mvol	168.890	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	574.95	K	Joback Method
tc	822.59	K	Joback Method
tf	428.31	K	Joback Method
vc	0.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.53	J/mol×K	574.95	Joback Method
cpg	484.88	J/mol×K	616.22	Joback Method
cpg	502.69	J/mol×K	657.50	Joback Method
cpg	519.60	J/mol×K	698.77	Joback Method
cpg	536.26	J/mol×K	740.04	Joback Method
cpg	553.31	J/mol×K	781.32	Joback Method
cpg	571.41	J/mol×K	822.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R617273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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